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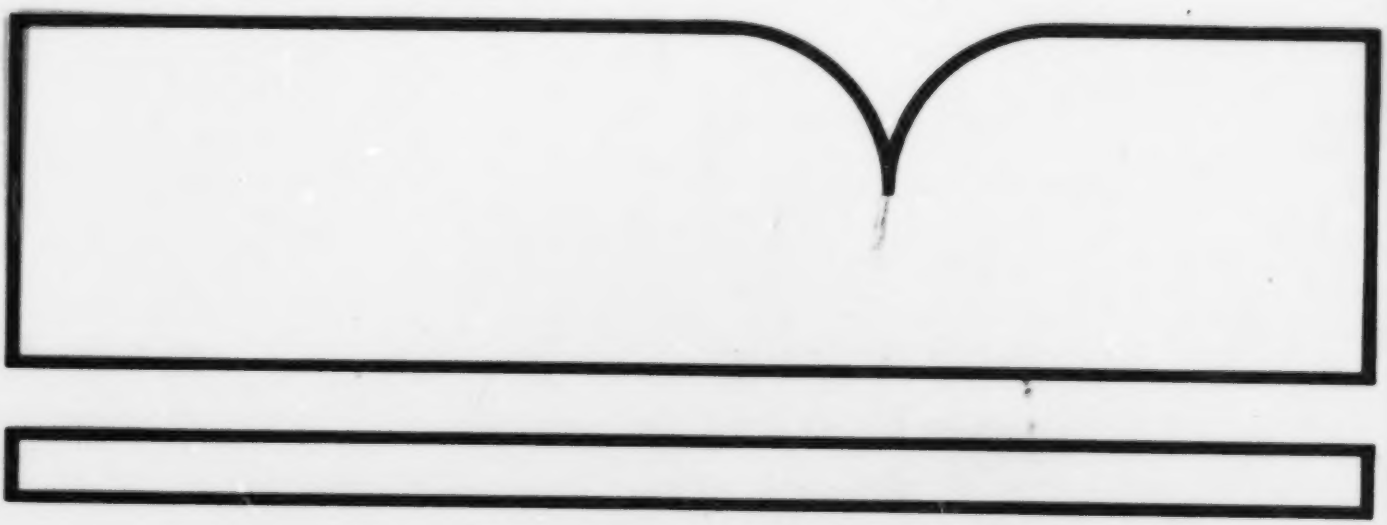

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Evaluation of the Empirical Kinetics Modeling Approach

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16. ABSTRACT

Describes four approaches used to evaluate the performance of the city-specific EKMA which has been recommended by EPA for use in 1982 State Implementation Plans.

Data included in graphs and tables depicts the results of actual experiments with each of the approaches: 1) comparison with historical trends, 2) impacts predicted with sophisticated models, 3) predicting peak ozone concentrations using a detailed database to estimate trajectories and 4) comparison with peak observed ozone concentrations using a minimal database and assumed trajectories.

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Introduction

The Empirical Kinetics Modeling Approach (EKMA) uses an ozone isopleth diagram (1) to estimate precursor controls needed to attain ambient air quality standards for ozone, or (2) to estimate the impact of specified reductions in ambient precursor levels on peak ozone concentrations. Isopleths used in EKMA are generated with a computer program called OZIPP (Ozone Isopleth Plotting Package).[1] When local data on meteorology, fresh emissions and pollutants transported from upwind sources are input to OZIPP, a set of "city-specific" ozone isopleths result. Use of city-specific isopleths in estimating the impact of precursor reductions is called "city-specific EKMA" or a "Level III analysis."[2]

City-specific EKMA has been recommended by the U.S. Environmental Protection Agency for use in 1982 State Implementation Plans (SIPs) as one means for estimating controls needed to attain the National Ambient Air Quality Standard (NAAQS) for ozone.[3] City-specific EKMA and its method of application have been described at length elsewhere.[4-6] It is sufficient to note here that the model represents a compromise between approaches having less physical basis and fewer data requirements (e.g., linear-rollback, envelope curves) and more rigorous approaches requiring extensive meteorological, air quality and emissions data (e.g., photochemical grid models). Given the resource constraints confronting many State and local agencies, it is clear why a relatively simple model like city-specific EKMA may be preferable to more rigorous approaches in many cases. However, the utility of city-specific EKMA for SIPs depends on how well such a simplified description is able to estimate the effectiveness of reducing precursor emissions. The purposes of this paper are:

(1) to describe approaches which have been used to evaluate the performance of city-specific EKMA, and

(2) to present the results of these evaluations.

Approaches for Evaluating City-Specific EKMA

The fundamental question in evaluating a model's performance in regulatory applications is, "If we control emissions as simulated in the model, will the air quality improve as predicted?" A more explicit form of this question applicable to ozone SIPs is: "If we reduce precursor emissions to the degree the model says is necessary to attain the ozone NAAQS, will the NAAQS be attained without overkill?" This question cannot be answered unequivocally, because historical observations of the necessary meteorological, air quality and emissions data are not available for a city which formerly experienced high ozone concentrations, has since applied controls, and now attains the NAAQS. Hence, there is no absolute "right" answer against which to compare model performance. The preceding limitation means that there is some unavoidable uncertainty regarding how accurately city-specific EKMA, or any other model for non-linear pollutants, performs in regulatory applications. Nevertheless, it is possible to indirectly assess the model's ability to accurately estimate reductions in precursors needed to attain the NAAQS for ozone.

Four approaches have been used to evaluate city-specific EKMA:

(1) comparison of model predictions with historical trends;

(2) comparison of impacts predicted with EKMA versus those predicted with "validated," more sophisticated photochemical models;

(3) comparison with peak observed ozone concentrations using a detailed data base to estimate trajectories;

(4) comparison with peak observed ozone concentrations using the minimal data base commensurate with city-specific EKMA and assumed trajectories.[2]

Approach 1: Comparison with Historical Trends

This approach is to: (1) review ambient ozone and precursor concentrations and emissions from a period prior to the implementation of major control programs; (2) note changes in ambient precursor levels and/or changes in emissions which have occurred over the period of record; (3) using either the observed changes in ambient precursors or emissions, estimate corresponding changes in ozone concentrations with the EKMA isopleths; (4) compare predicted changes in ozone with those actually observed.

Because it comes closest to directly evaluating the model's ability to simulate the impact of regulatory controls, Approach 1 is the most intuitively appealing of the four approaches. Unfortunately, there are several limitations. First, if there are insufficient ambient precursor data, there may be uncertainty about whether emission reductions claimed are actually realized. Second, only the Los Angeles Basin has a sufficiently long period of record for the technique to be used. Third, information on NMOC/NO_x ratios (a key input to EKMA) prevailing in the mid-sixties in Los Angeles must be arrived at indirectly, thereby introducing uncertainty. Finally, even though a vigorous control program has been in effect in the Los Angeles Basin, this has apparently been counteracted by the large growth experienced in the area over the past 15-20 years. The net result is that the reductions in ambient precursor levels and estimated emissions are small, as is the reduction in observed ozone. One would not expect to find a wide divergence between model predictions and observations under such circumstances.

Approach 2: Comparison of Control Strategies Simulated City-Specific EKMA and with More Sophisticated Photochemical Models

This approach is to: (1) run sophisticated photochemical models for a limited number of days in a city; (2) satisfy oneself that the sophisticated models agree with observations; (3) simulate a control strategy with the sophisticated model; (4) simulate the same strategy with EKMA and see how well the results agree with those in step (3).

Use of validated photochemical dispersion models which explicitly treat the chemical and physical processes affecting ozone concentrations represents the best estimate we are able to make of the impact of control strategies. Therefore, if the impacts of control strategies predicted with city-specific EKMA are similar to those obtained with more complex models, estimates obtained with city-specific EKMA are about as good as the state of the art permits. A major advantage that Approach 2 has over direct comparison of EKMA with trends is that many more comparisons can be made simulating a variety of control strategies under differing meteorological conditions.

There are two shortcomings with Approach 2. First, it does not necessarily follow that close agreement between a sophisticated model and observations prior to the initiation of controls will continue after controls have been applied. That is, there is no guarantee that the sophisticated models provide the "correct" answer. Second, predictions obtained with sophisticated models do not always agree with observations. The underlying reasons for this lack of consistent agreement are not yet clear. In the comparisons between sophisticated models and EKMA, only cases in which predictions of peak ozone obtained with sophisticated models agree within 30% of observed peaks are reported herein.

Approach 3: Comparison with Air Quality Observations Using a Detailed Data Base to Estimate Trajectories

This approach is to: (1) select a limited number of days for which there are detailed emissions, meteorological and air quality data; (2) use these data to derive detailed trajectories; (3) using derived trajectories, apply a more flexible version of OZIPP to estimate peak ozone; (4) compare predicted and observed peak ozone concentrations.

Approach 3 is similar to approaches used to "verify" sophisticated models. If a model is able to successfully simulate existing conditions without extensive tuning, this inspires confidence in its usefulness for regulatory applications. In order for such an exercise to be most meaningful, use of detailed wind field data and spatially disaggregated emission inventories are needed. In effect, a "Level II" analysis is performed.[2] Hence, a more extensive data base than that required by city-specific EKMA is used.

There are several difficulties with Approach 3. First, as with more sophisticated models, there is no guarantee that if the model works well in simulating the base case, it will do as well in simulating conditions after the implementation of controls. Second, EKMA uses observed rather than predicted ozone concentrations as a starting point for estimating control requirements. Failure to predict peak ozone concentrations closely does not necessarily mean EKMA predicts the impact of controls inaccurately. Hence, Approach 3 is a less direct test of the model's usefulness for regulatory applications than Approaches 1 and 2.

Approach 4: Comparison with Air Quality Observations Using Data Base Commensurate with City-Specific EKMA and Assumed Trajectories

Approach 4 is to: (1) consider a countywide emissions inventory and assume a trajectory in which an air parcel starts from center city at 8 a.m. and reaches the site of the observed maximum ozone concentration at the time of the observed maximum; (2) use the information in (1) in OZIPP to predict the peak ozone concentration; (3) compare predicted and observed maximum ozone concentrations.

The rationale underlying Approach 4 rests on two bases. First, the size of the data base used is consistent with that likely with city-specific EKMA. Second, it became clear in applying Approach 3 that a consistent wind field is very difficult to define, even with a large number of monitors and measurements aloft. In the end, significant uncertainties exist with derived trajectories, even when sophisticated techniques are used for their development. Approach 4 simply assumes that the observed peak ozone is largely produced from precursors found within the city in the early morning or emitted subsequently. No attempt is made to define an exact trajectory. Spatial detail in the emission inventory is consistent with the lack of detail in the wind field. A priori, one might expect Approach 4 to overestimate observed ozone. The sparse network of ozone monitors may not detect the maximum ozone level which actually occurs in a city. Further, the assumed trajectory tends to maximize the impact of the city.

There are two disadvantages with Approach 4. First, like Approach 3, it is not a direct test of the model's ability to accurately predict the impact of control strategies. Second, it is less rigorous than Approach 3. As such, there is a greater likelihood that agreement between observations and predictions is fortuitous.

Results

Each of the four approaches described in the previous section has been exercised at least once. Table I indicates the locations and data bases used in performing the various tests.

Approach 1: Comparison with Trends

City-specific ozone isopleths have been generated for Los Angeles and compared with trends observed between 1964 and 1978.[7] These comparisons differ from those reported previously by Trijonis and Hunsaker.[10] The comparisons described herein consider the impact of midday precursor emissions and are believed to more accurately reflect atmospheric dilution observed on days with high ozone. Two trend parameters are examined in the most recent studies: the 95th percentile value of daily maximum ozone concentrations and the maximum ozone value observed each year. To dampen effects of variable meteorology, predicted changes are compared with observed changes using running three year averages of the observed trend parameters. This procedure is illustrated in Figure 1.[7]

Figure 1 actually shows the results of four independent comparisons. For example, results of the comparison for 1971 are not in any way affected by the results obtained for 1968. Comparisons similar to those in Figure 1 have been performed at three additional sites in the Los Angeles basin. In addition, four comparisons between changes in observed and predicted basinwide maximum ozone concentrations have been made. As a result, a total of 16 (i.e., 4 comparisons at 4 sites) comparisons exist using the 95th percentile maximum daily ozone trend parameter. Twenty comparisons (i.e., 4 comparisons at 4 sites, plus 4 comparisons between observed and predicted basinwide maximums) exist for the maximum ozone trend parameter. Predictions have been made using trends in observed precursor levels and using estimated trends in emissions. The results of these comparisons are presented in Table II(a).

Table II(a) suggests that about 60-80% of the predictions agree with observations within rather narrow bands of uncertainty attributable to smoothing three-year average values for observed ozone trend parameters and spatial differences in precursor trends input to the model. However, additional uncertainty exists about NMOC/NO_x ratios prevailing in the Los Angeles Basin during the mid-1960's. No measurements are available. Therefore, estimates of the ratio are arrived at by considering emissions reductions alleged to have occurred during the 1960's. Although the 25:1 and 7:1 limits in Figure 2 are perhaps too wide, they indicate the effect uncertainty in prevailing NMOC/NO_x ratio has on EKMA predictions. Even with somewhat narrower uncertainty bands, all predictions and observations agree when uncertainty in NMOC/NO_x ratio is considered.

Approach 2: Comparison with Other Models

A total of 33 comparisons between city-specific EKMA and a variety of more sophisticated models (shown in Table I) are available. Each strategy simulated with EKMA and one of the other models constitutes a comparison. Table III exemplifies several such comparisons. Note from Table III that whenever the absolute value of change in ozone predicted with EKMA is greater than the change predicted with another model, the difference is expressed as a positive number. The histogram in Figure 3 represents the actual distribution of differences for all comparisons. This has been approximated by a normal distribution whose parameters are also shown in Figure 3. For the available sample, results in Figure 3 suggest that city-specific EKMA provides an unbiased indicator of what sophisticated models would predict to be the impact of various control strategies. Twenty-six (26) of the 33 comparisons are within 10% of one another.

A principal concern with the use of city-specific EKMA is that it not be used to prescribe overly stringent controls. If it is assumed that sophisticated models provide the best possible predictions, focussing on the left-hand tail of the distribution in Figure 3 allows one to assess the likelihood of underestimating the impact of controls using EKMA. Using a model which underestimates the impact of controls would, in effect, cause an analyst to prescribe controls which are too stringent. Probabilities of underestimating the impact of controls are listed in Table IV.

Approach 3: Comparison with Air Quality Data Using a Detailed Data Base

A total of 16 comparisons are available between predicted and observed peak hourly ozone concentrations using the detailed trajectories of Approach 3. Of these, ten agree within ±30%. As seen in Figure 4, there is a tendency for predictions to underestimate observations. This is more obvious if the San Francisco comparisons are disregarded. At present, efforts to understand reasons for the tendency to underpredict in St. Louis and Los Angeles are incomplete. In St. Louis, there appears to be some correspondence between poor model performance and ambiguous data concerning wind flow. In Los Angeles, the day in which the model performs most poorly is the second day of a two day episode. Several more sophisticated models also performed poorly on this day.[8] One possible explanation may be that incorrect initial and boundary conditions were assumed as input to the models.

Comparison with Air Quality Observations Using a Data Base Commensurate with City-Specific EKMA

Ten comparisons have been made for the same days in St. Louis as those shown in Figure 4. A typical data base used with city-specific EKMA requires one to assume an air parcel follows a straight line trajectory between center city and the site observing the maximum ozone concentration. As described previously, such a trajectory tends to maximize the predicted impact of a city. The results of comparisons obtained using Approach 4 are shown in Figure 5. It is clear from comparing the positions of the numbered points in Figures 4 and 5 that EKMA appears to perform better when Approach 4 is used instead of Approach 3. Predictions are only slightly low, with eight of ten comparisons agreeing within ±30% of observations. Because of the dense monitoring network utilized during the St. Louis RAPS, observations are not likely to underestimate the "true maximum" value. Hence, the close and only slightly biased predictions in Figure 5 are encouraging.

Summary and Implications

Key performance criteria for a model in regulatory applications are (1) "how accurately does it prescribe controls needed to attain the NAAQS"?, and (2) "how well does it predict the impact of control strategies?" Unfortunately, there is no way to provide an unequivocal evaluation of city-specific EKMA using these criteria. Four approaches have been investigated. Comparisons to date indicate (1) agreement with historical trends, subject to considerable uncertainty; (2) general agreement with impacts predicted with sophisticated models; (3) a tendency to underpredict peak ozone concentrations using detailed trajectories and data bases; and (4) generally good agreement with observed peak ozone concentrations using assumed trajectories with a commensurate data base.

The results, on balance, indicate the model will probably perform adequately most of the time. Comparison with complex model estimates (Approach 2) and with air quality data using an assumed trajectory (Approach 4) suggest city-specific EKMA may serve as an adequate predictor, given the amount of air quality, meteorological and emissions data typically available to State agencies. Experience with model evaluations using a detailed data base (Approach 3) suggests that, at the present stage of model development, it may not be particularly fruitful to run city-specific EKMA in a manner which is more sophisticated than suggested in EPA Guidelines.[6]

It is also apparent that there is unavoidable uncertainty associated with the model's predictions. For example, the model performs better on some days and locations than for others. Further, although there is general agreement with estimates obtained with more sophisticated models, discrepancies are occasionally found. The uncertainty in model predictions tends to emphasize the need for modeling several days in each city. Such a procedure is also consistent with existing guidance for demonstrating attainment of the NAAQS for ozone.[6]

Acknowledgements

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Table I. Summary of EKMA Evaluation Studies

City	Approach 1	Approach 2	Approach 3	Approach 4	Data Base
Los Angeles	A	B (SAI Trajectory)	C		A - AQ - emissions data 1964-78[7] B - Two days: June 26, 1974, August 4, 1975[8] C - Three days: June 26-27, 1979; August 4, 1975[8]
St. Louis		D (SAI Airshed)	E	E	D - Three days during 1976 RAPS E - Nine days during 1976 RAPS
Sacramento		F (SAI Trajectory)			F - One hypothetical day[9]
San Francisco		G (LIRAQ)	H		G - One day, July 26, 1973[9] H - Three days: July 26, August 20, 1973 July 24, 1974

Table II. Summary of Los Angeles Trend Comparisons*

	Trend Parameters	
	95th Percentile	Maximum Ozone
	(a)	
Using Ambient Precursor Trends	12/16	14/20
Using Emissions Trends	10/16	13/20
	(b)	
Including Uncertainty in NMOC/NO_x Ratio	16/16	20/20

* numerator = cases of agreement within uncertainty bounds

demoninator = number of comparisons

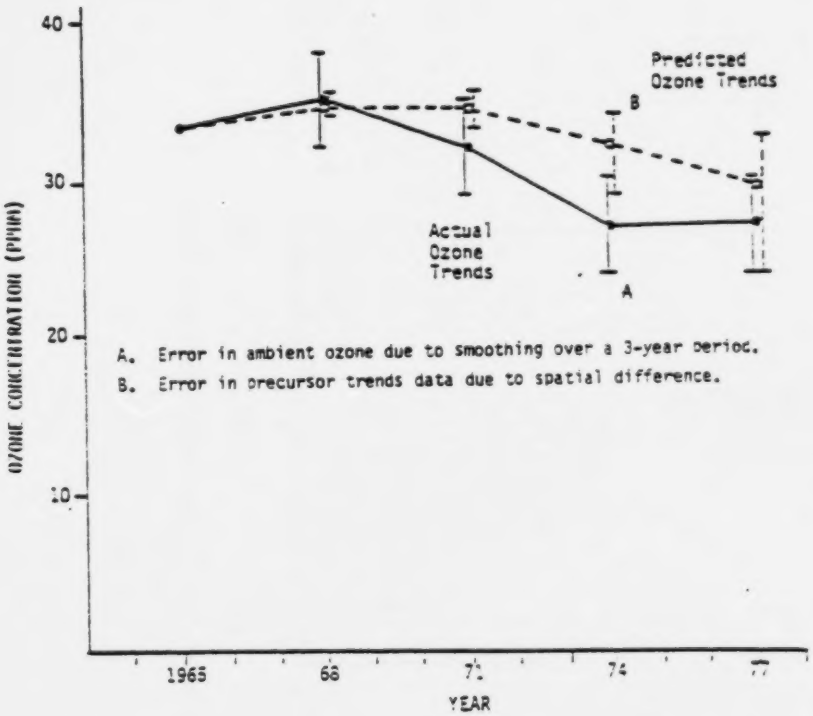
Table IV. Probability of Underestimating Impact of Controls

Size of Underestimate	Likelihood
$\geq$ 20%	1/100
$\geq$ 15%	1/27
$\geq$ 10%	1/9
$\geq$ 5%	1/4

Table III. Example Set of Comparisons Between EKMA and Another Model for St. Louis*

Date 7/13/76									
	%ΔNMOC	+67	+17	-17	-42	-63	0	-42	-42
	$\%\Delta NO_x$	0	0	0	0	0	+20	+20	-20
% ΔO_3	Airshed Model	+16	+6	-8	-26	-50	-1	-38	-20
	City-Specific EKMA	+15	+6	-8	-28	-57	+3	-37	-25
Difference in Sensitivity (EKMA - Airshed)		-1	0	0	+2	+7	+2	-1	+5

* changes and differences all expressed in %.



A. Error in ambient ozone due to smoothing over a 3-year period.
B. Error in precursor trends data due to spatial difference.

Figure 1. Results of the validation studies for the 95th percentile of daily maximum ozone at Azusa, using emission trends to derive predicted ozone trends.

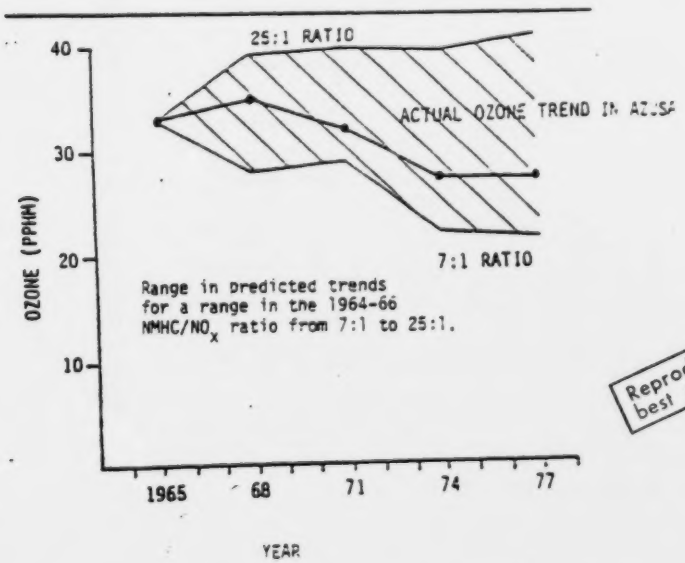


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Figure 2. Uncertainty introduced by uncertainty in $NMOC/NO_x$ ratio in Los Angeles during the 1960's.

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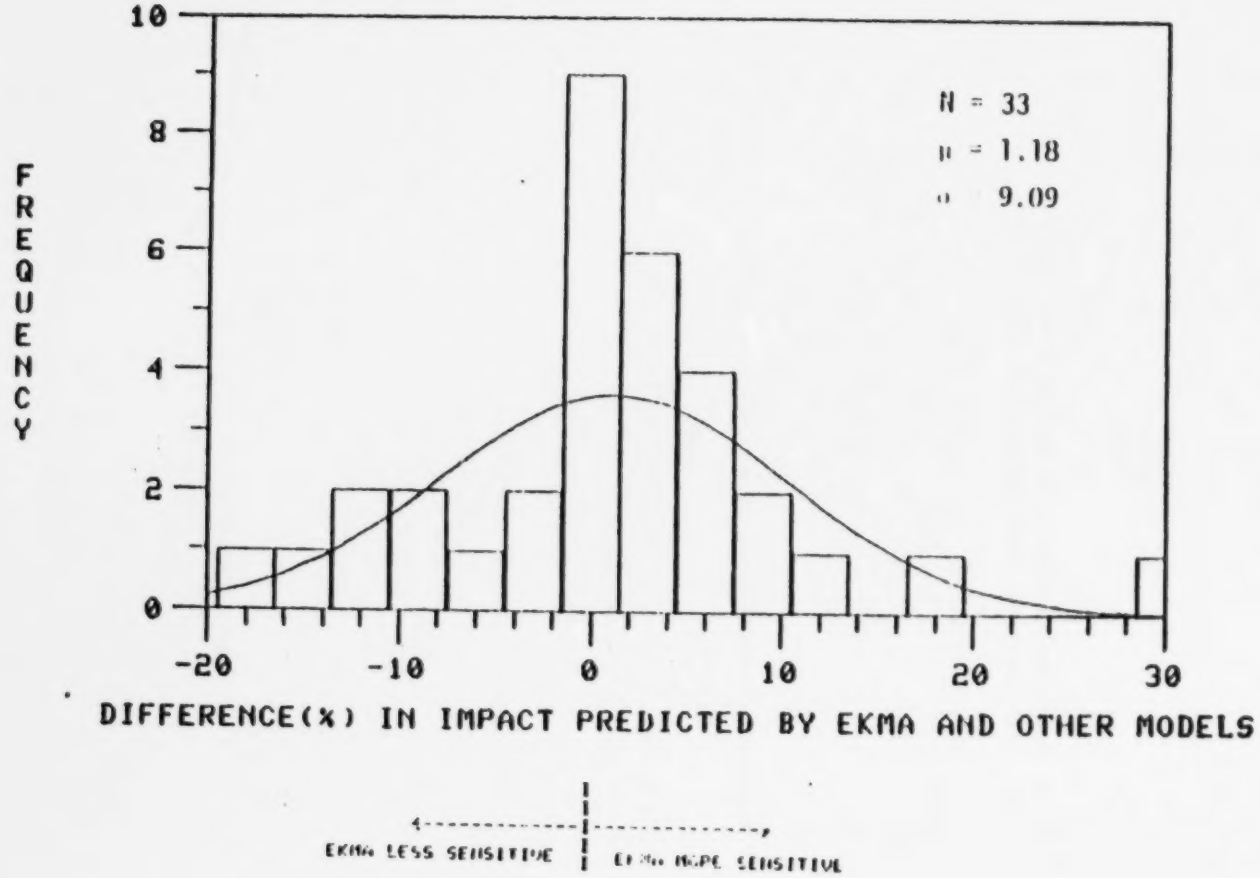

FIGURE 3. DISTRIBUTION OF DIFFERENCES BETWEEN CITY-SPECIFIC EKMA AND OTHER MODELS

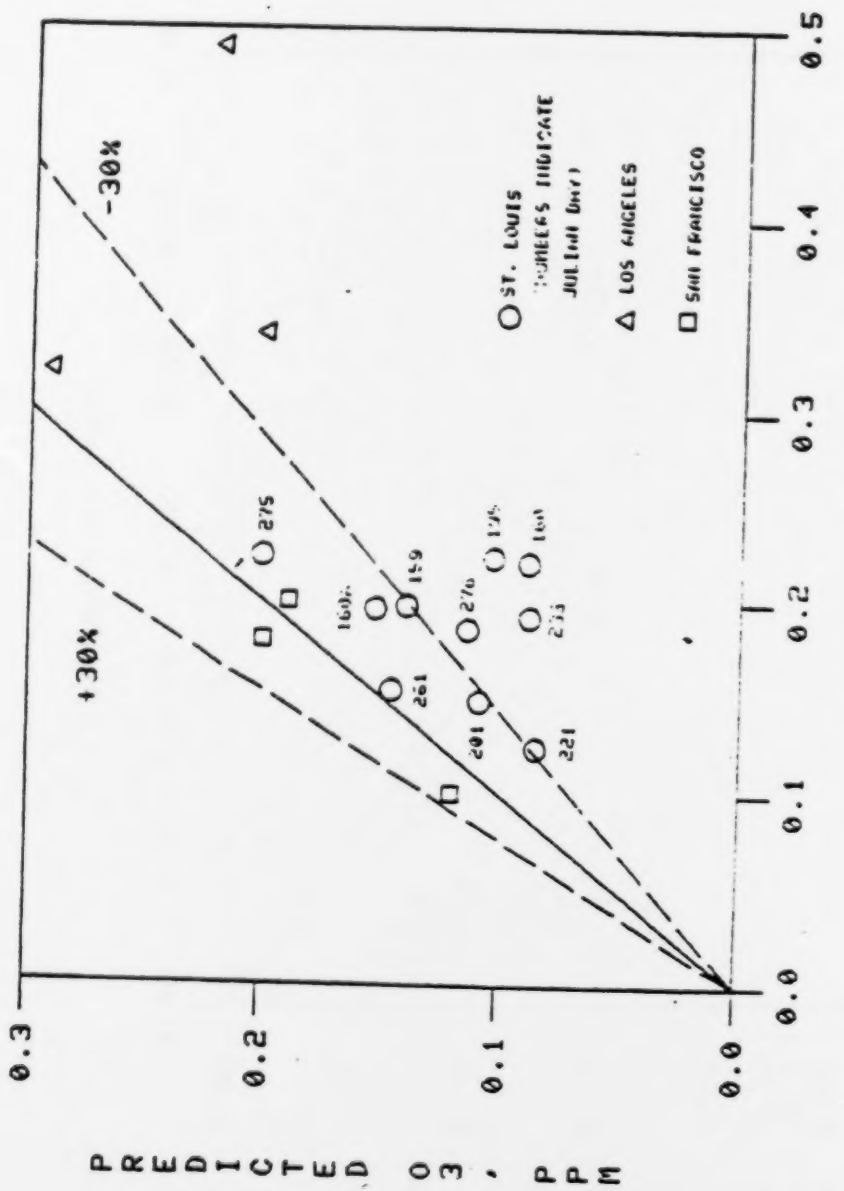

FIGURE 4. LEVEL II EKMA VS. AIR QUALITY

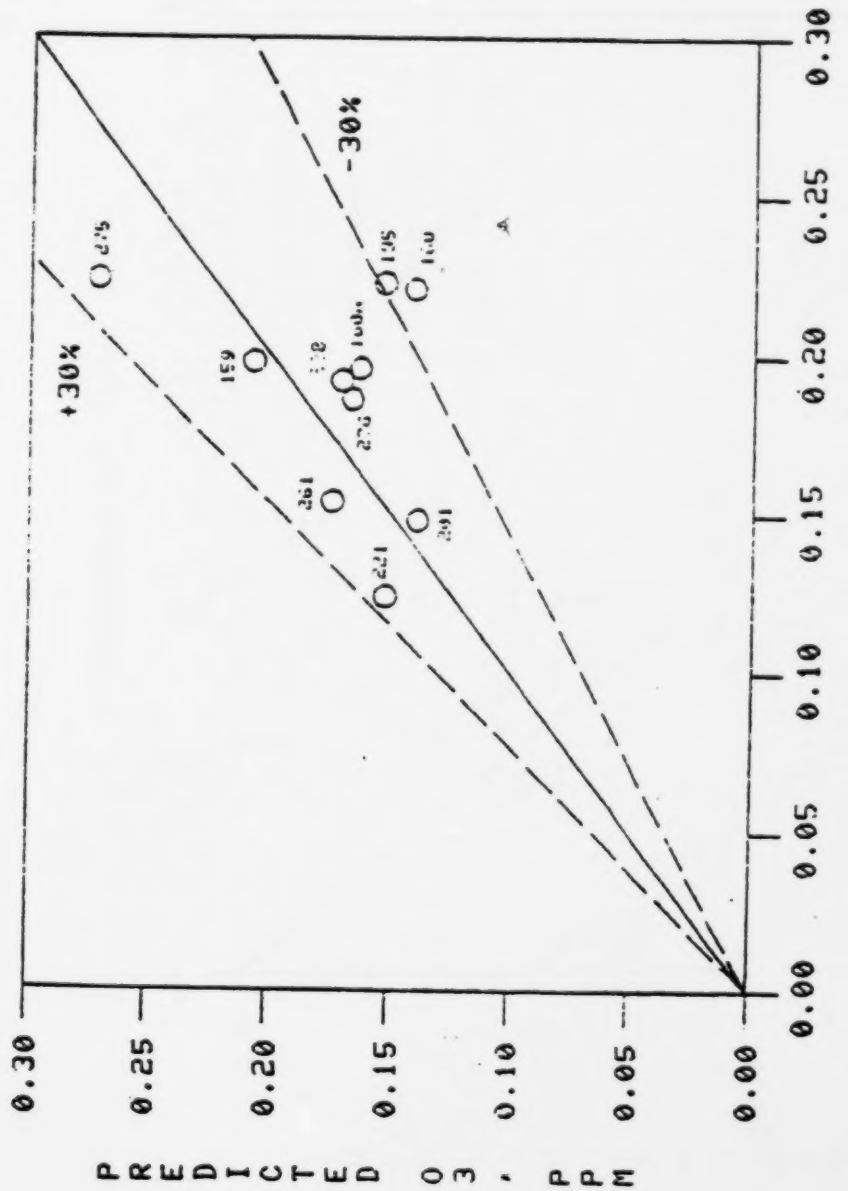

FIGURE 5. LEVEL III EKMA VS. AIR QUALITY

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